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Microwave spectrum and electric dipole moment of cyclopentanone

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In the present investigation 14 rotational transitions in the absorbtion spectrum of cyclopentanone (C_5H_8O) have been measured. Some of these lines have not been previously reported. The rotational constants were calculated and found to be in reasonable agreement with those obtained by Erlandsson [1] and Burkhalter [2]. From studies of the Stark effect of certain lines we have found the value (3.30 ± 0.01) Debye units for the electric dipole moment of the molecule, measured in the gaseous state.

The measurements were made by the aid of the Stark effect modulated microwave spectrometer described by Erlandsson [3]. The frequency-range, however, has been extended by means of a new klystron (type Varian X-13) and a simple taper section to make it possible to measure the two lines below the earlier frequency range of the described apparatus.

Table 1.

Transition	ν_{calc} (MHz)	ν_{obs} (MHz)
1_{01}–2_{02}	11348.6	11349.1
1_{11}–2_{12}	10582.7	10582.3
1_{10}–2_{11}	12465.4	12465.9
2_{02}–3_{03}	16621.1	16621.8
2_{12}–3_{13}	15773.0	15773.9
2_{11}–3_{12}	18576.2	18576.2
2_{21}–3_{22}	17286.1	17286.7
2_{20}–3_{21}	17951.1	17950.7
3_{03}–4_{04}	21569.4	21568.5
3_{13}–4_{14}	20868.4	20868.2
3_{12}–4_{13}	24511.5	24510.9
3_{22}–4_{23}	22910.5	22910.0
3_{21}–4_{22}	24387.2	24387.2
3_{31}–4_{32}	23345.2	23346.0

The transitions measured are given in table 1. The electronic computer BESK was used to calculate the rotational constants in the manner described in [3]. The values obtained for the rotational parameters are $A = 6.62453$ MHz, $B = 3.35169$ MHz, $C = 2.41035$ MHz, $\varkappa = -0.55325$.

Table 2.

Transition	M (magnetic quantum number)	$\frac{\Delta \nu^*}{E^2}$ ($\Delta \nu$ in MHz E in e.s.u.)	μ^* (Debye)
2_{02}–3_{03}	2	2.17 ± 0.09	3.33 ± 0.07
2_{11}–3_{12}	1	1.94 ± 0.02	3.29 ± 0.02
	2	6.99 ± 0.09	3.31 ± 0.02
2_{21}–3_{22}	1	146 ± 8	3.26 ± 0.09

* r.m.s. error given.

The rather large discrepancies between the observed and calculated frequencies are probably due to uncertainties caused by the line widths which for most of the lines were considerable.

The Stark effect splittings $\Delta \nu$ for some of the lines were studied for different field strengths E in the Stark cell (i.e. for different voltages applied to the electrode). The measurements of the splittings were difficult because of disturbances from adjacent lines, probably caused by low excited vibrational states. For a few lines, however, it was possible to follow certain Stark effect components over a reasonable voltage range. The quotient $\Delta \nu / E^2$ for these components is given in table 2 as a mean value from several measurements with different voltages. From these quotients the dipole moment of the molecule was calculated in the manner described in (4). For the present molecule, however, the dipole moment is assumed to be directed along the axis of least moment of inertia. The obtained values of the dipole moment are given in table 2. For some other lines it was only possible to make rough estimations which don't disagree, however, with the abovementioned quantitative determinations. From the values given in the table we obtain a mean value for the dipole moment of (3.30 ± 0.01) Debye units. If the maximum observed errors are considered, the value (3.30 ± 0.15) Debye units may be given.

The values of the dipole moment previously given in the literature, for example 3.00 Debye units (5), are considerably lower than our result. As those values are obtained from measurements on solutions, the difference may be due to solvent effects.

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